



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:54 am GMT

PDB ID : 1WAJ  
Title : DNA POLYMERASE FROM BACTERIOPHAGE RB69  
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Steitz, T.A.  
Deposited on : 1997-04-13  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

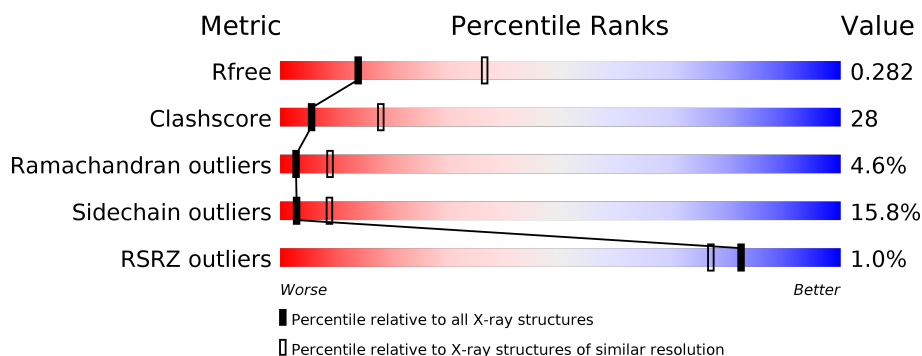
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	903	<div> <div></div> <div>47%</div> <div>42%</div> <div>9%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

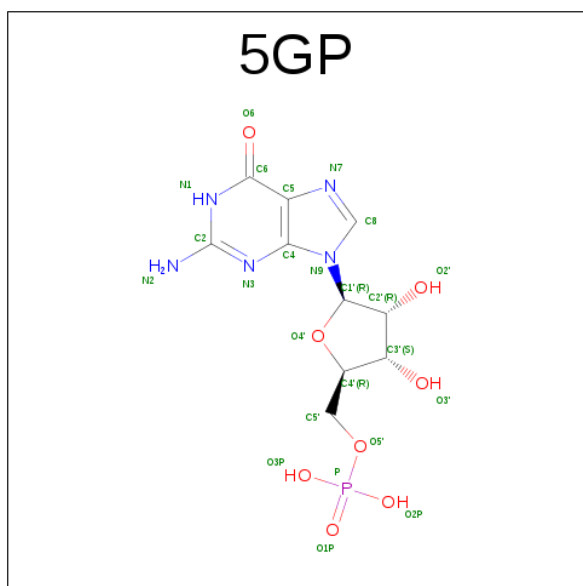
There are 3 unique types of molecules in this entry. The entry contains 7465 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	0	0
			7380	4739	1226	1382	33			

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula:  $C_{10}H_{14}N_5O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	4	0
			24	10	5	8	1		

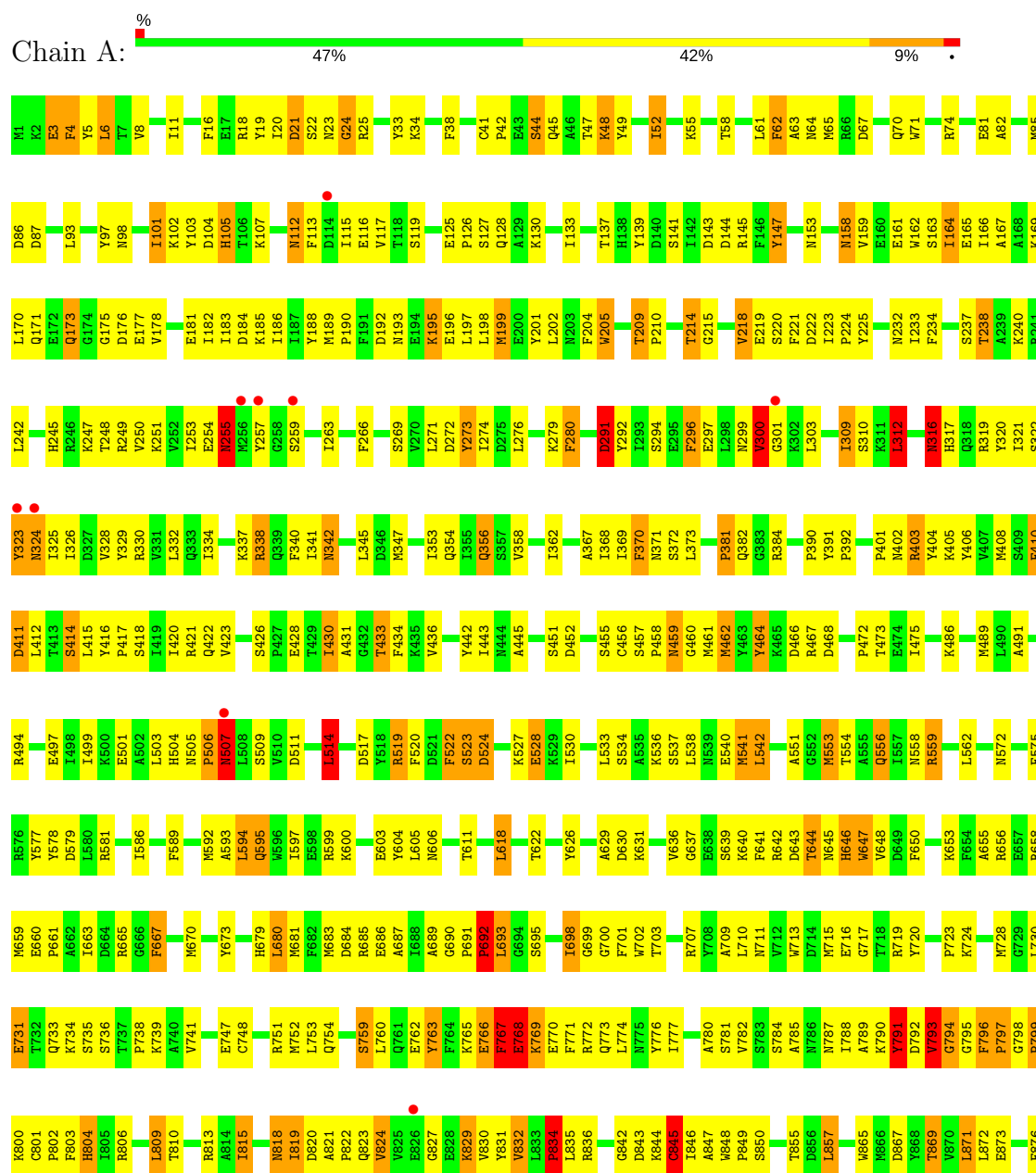
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	61	Total 61 O 61	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: DNA POLYMERASE



L880	L881	L882	F883	T884	L885	L886	L887	L888	L889	D890	Y891	E892	X893	X894	L897	F898	D899	M900	F901	D902	F903
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.41Å 117.60Å 199.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 29.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.80) 86.0 (29.89-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.80Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.210 , 0.280 0.223 , 0.282	Depositor DCC
$R_{free}$ test set	2092 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5GP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.73	6/7561 (0.1%)	0.86	10/10217 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	SER	CB-OG	-6.39	1.33	1.42
1	A	220	SER	CB-OG	-5.55	1.35	1.42
1	A	269	SER	CB-OG	-5.38	1.35	1.42
1	A	294	SER	CB-OG	-5.21	1.35	1.42
1	A	414	SER	CB-OG	-5.19	1.35	1.42
1	A	759	SER	CB-OG	-5.16	1.35	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	PHE	N-CA-C	7.62	131.58	111.00
1	A	48	LYS	N-CA-C	-7.51	90.71	111.00
1	A	101	ILE	N-CA-C	7.07	130.08	111.00
1	A	794	GLY	N-CA-C	-6.21	97.57	113.10
1	A	680	LEU	N-CA-C	5.96	127.08	111.00
1	A	62	PHE	N-CA-C	5.90	126.93	111.00
1	A	692	PRO	N-CA-C	5.20	125.63	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	LEU	N-CA-C	5.04	124.59	111.00
1	A	767	PHE	N-CA-C	-5.03	97.43	111.00
1	A	768	GLU	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7380	0	7265	417	0
2	A	24	0	12	0	0
3	A	61	0	0	12	0
All	All	7465	0	7277	417	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (417) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ILE:HG22	1:A:254:GLU:H	1.05	1.07
1:A:253:ILE:HG22	1:A:254:GLU:N	1.74	1.01
1:A:752:MET:HG2	1:A:760:LEU:HD12	1.45	0.98
1:A:253:ILE:CG2	1:A:254:GLU:H	1.80	0.94
1:A:52:ILE:HD13	1:A:52:ILE:H	1.32	0.93
1:A:643:ASP:HB3	1:A:646:HIS:HB3	1.52	0.91
1:A:431:ALA:HA	1:A:464:TYR:HE1	1.39	0.88
1:A:188:TYR:HE1	1:A:190:PRO:HG3	1.37	0.88
1:A:116:GLU:HG3	1:A:324:ASN:HD21	1.39	0.87
1:A:597:ILE:HB	1:A:667:PHE:HE1	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HD13	1:A:16:PHE:HD2	1.41	0.85
1:A:791:TYR:OH	1:A:801:CYS:HA	1.77	0.84
1:A:254:GLU:O	1:A:255:ASN:HB2	1.78	0.81
1:A:214:THR:HG22	1:A:215:GLY:H	1.44	0.80
1:A:356:GLN:NE2	1:A:356:GLN:H	1.79	0.80
1:A:356:GLN:HE21	1:A:356:GLN:H	1.29	0.80
1:A:214:THR:HG21	1:A:273:TYR:HD2	1.48	0.79
1:A:830:VAL:HG12	1:A:831:TYR:N	1.97	0.79
1:A:832:VAL:HA	1:A:846:ILE:O	1.81	0.79
1:A:233:ILE:HG13	1:A:234:PHE:CD1	2.17	0.79
1:A:643:ASP:HB3	1:A:646:HIS:CB	2.14	0.78
1:A:511:ASP:HB2	3:A:905:HOH:O	1.82	0.77
1:A:162:TRP:HB3	1:A:188:TYR:CE2	2.20	0.77
1:A:667:PHE:CE2	1:A:681:MET:HB3	2.19	0.76
1:A:330:ARG:O	1:A:334:ILE:HG13	1.85	0.76
1:A:34:LYS:HD2	1:A:63:ALA:HA	1.66	0.76
1:A:647:TRP:CD1	1:A:648:VAL:N	2.54	0.76
1:A:700:GLY:HA3	1:A:710:LEU:HD23	1.67	0.76
1:A:663:ILE:HG21	1:A:683:MET:HE2	1.69	0.73
1:A:405:LYS:HA	1:A:698:ILE:O	1.88	0.72
1:A:834:PRO:O	1:A:835:LEU:HB2	1.87	0.72
1:A:522:PHE:O	1:A:523:SER:HB3	1.88	0.71
1:A:809:LEU:O	1:A:813:ARG:HG3	1.90	0.71
1:A:739:LYS:HG2	3:A:951:HOH:O	1.90	0.71
1:A:272:ASP:OD1	1:A:274:ILE:HG22	1.90	0.71
1:A:356:GLN:HE21	1:A:356:GLN:N	1.87	0.71
1:A:713:TRP:CZ3	1:A:723:PRO:HG3	2.25	0.71
1:A:193:ASN:HD21	1:A:195:LYS:HB2	1.57	0.70
1:A:489:MET:SD	1:A:553:MET:CB	2.79	0.70
1:A:52:ILE:CD1	1:A:52:ILE:H	2.03	0.70
1:A:218:VAL:HG13	1:A:223:ILE:HD11	1.73	0.70
1:A:830:VAL:HG11	1:A:847:ALA:HB1	1.73	0.70
1:A:52:ILE:N	1:A:52:ILE:HD13	2.07	0.70
1:A:796:PHE:CD2	1:A:797:PRO:HD2	2.27	0.70
1:A:41:CYS:SG	1:A:45:GLN:HG3	2.32	0.69
1:A:796:PHE:HD2	1:A:797:PRO:HD2	1.56	0.69
1:A:830:VAL:HG12	1:A:831:TYR:H	1.58	0.69
1:A:830:VAL:CG1	1:A:847:ALA:HB1	2.22	0.69
1:A:489:MET:SD	1:A:553:MET:HB3	2.33	0.69
1:A:597:ILE:HD13	1:A:667:PHE:HD1	1.58	0.68
1:A:404:TYR:CZ	1:A:618:LEU:HD21	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLN:N	1:A:173:GLN:HE21	1.91	0.68
1:A:597:ILE:HD13	1:A:667:PHE:CD1	2.28	0.68
1:A:128:GLN:HE21	1:A:130:LYS:HD2	1.58	0.67
1:A:653:LYS:HD2	1:A:656:ARG:NH1	2.10	0.67
1:A:504:HIS:O	1:A:506:PRO:HD3	1.94	0.67
1:A:205:TRP:HZ3	1:A:242:LEU:O	1.77	0.66
1:A:499:ILE:HG21	1:A:542:LEU:HB2	1.77	0.66
1:A:188:TYR:CE1	1:A:190:PRO:HG3	2.26	0.66
1:A:788:ILE:HG22	1:A:791:TYR:HB3	1.77	0.66
1:A:403:ARG:NH1	1:A:888:LYS:HB2	2.10	0.66
1:A:145:ARG:HD3	1:A:185:LYS:O	1.96	0.66
1:A:341:ILE:O	1:A:345:LEU:HD23	1.96	0.66
1:A:663:ILE:HD13	1:A:683:MET:CE	2.26	0.66
1:A:846:ILE:HG22	1:A:847:ALA:N	2.11	0.66
1:A:21:ASP:OD1	1:A:25:ARG:HB2	1.96	0.65
1:A:507:ASN:HA	1:A:534:SER:HA	1.79	0.65
1:A:431:ALA:HA	1:A:464:TYR:CE1	2.26	0.65
1:A:788:ILE:O	1:A:791:TYR:HD2	1.79	0.65
1:A:834:PRO:HB3	1:A:867:ASP:HB3	1.79	0.65
1:A:734:LYS:HG3	3:A:943:HOH:O	1.96	0.65
1:A:280:PHE:CD1	1:A:280:PHE:N	2.64	0.64
1:A:422:GLN:HE22	1:A:681:MET:HG2	1.62	0.64
1:A:530:ILE:HA	1:A:533:LEU:HD23	1.80	0.64
1:A:738:PRO:HB2	1:A:741:VAL:HG23	1.79	0.64
1:A:787:ASN:C	1:A:789:ALA:H	1.99	0.64
1:A:593:ALA:HA	1:A:670:MET:CE	2.28	0.64
1:A:147:TYR:CD1	1:A:147:TYR:N	2.65	0.63
1:A:112:ASN:HD22	1:A:112:ASN:C	2.01	0.63
1:A:459:ASN:HD22	1:A:459:ASN:H	1.46	0.63
1:A:748:CYS:O	1:A:752:MET:HG3	1.98	0.63
1:A:296:PHE:CD1	1:A:296:PHE:C	2.68	0.63
1:A:81:GLU:HB2	3:A:924:HOH:O	1.98	0.63
1:A:414:SER:O	1:A:417:PRO:HD2	1.99	0.62
1:A:408:MET:HE1	1:A:655:ALA:HB2	1.81	0.62
1:A:280:PHE:N	1:A:280:PHE:HD1	1.97	0.62
1:A:8:VAL:HG11	1:A:93:LEU:HD21	1.80	0.62
1:A:219:GLU:HA	1:A:223:ILE:HD12	1.81	0.62
1:A:491:ALA:HB3	1:A:519:ARG:O	2.00	0.62
1:A:489:MET:SD	1:A:553:MET:HB2	2.39	0.62
1:A:434:PHE:CE2	1:A:460:GLY:HA2	2.35	0.61
1:A:644:THR:HB	1:A:692:PRO:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.83	0.61
1:A:33:TYR:HB3	1:A:65:MET:HE3	1.82	0.61
1:A:752:MET:CG	1:A:760:LEU:HD12	2.26	0.61
1:A:647:TRP:O	1:A:650:PHE:HB3	1.99	0.61
1:A:830:VAL:CG1	1:A:831:TYR:N	2.64	0.61
1:A:4:PHE:HD1	1:A:4:PHE:N	1.99	0.61
1:A:794:GLY:C	1:A:796:PHE:H	2.01	0.61
1:A:846:ILE:HG22	1:A:847:ALA:H	1.66	0.60
1:A:581:ARG:HH11	1:A:581:ARG:HG3	1.66	0.60
1:A:667:PHE:HE2	1:A:681:MET:HB3	1.64	0.60
1:A:785:ALA:C	1:A:787:ASN:H	2.04	0.60
1:A:647:TRP:HH2	1:A:691:PRO:O	1.84	0.60
1:A:391:TYR:HB2	1:A:392:PRO:HD2	1.84	0.60
1:A:3:GLU:HB2	1:A:20:ILE:O	2.02	0.60
1:A:685:ARG:HG2	1:A:686:GLU:N	2.16	0.60
1:A:824:VAL:HA	3:A:920:HOH:O	2.02	0.60
1:A:316:ASN:HD22	1:A:316:ASN:C	2.05	0.60
1:A:11:ILE:HD13	1:A:16:PHE:CD2	2.31	0.60
1:A:188:TYR:O	1:A:189:MET:HG3	2.02	0.59
1:A:362:ILE:HD11	1:A:572:ASN:HB3	1.84	0.59
1:A:328:VAL:O	1:A:332:LEU:HD23	2.03	0.59
1:A:831:TYR:CE2	1:A:850:SER:HA	2.36	0.59
1:A:342:ASN:O	1:A:345:LEU:HB2	2.03	0.59
1:A:445:ALA:HA	1:A:673:TYR:CE2	2.38	0.58
1:A:4:PHE:CD1	1:A:4:PHE:N	2.71	0.58
1:A:835:LEU:HD21	1:A:846:ILE:HG13	1.84	0.58
1:A:162:TRP:HB3	1:A:188:TYR:HE2	1.67	0.58
1:A:279:LYS:C	1:A:280:PHE:HD1	2.07	0.58
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.85	0.58
1:A:685:ARG:NH2	1:A:717:GLY:H	2.00	0.57
1:A:667:PHE:CD2	1:A:681:MET:HB3	2.39	0.57
1:A:803:PHE:O	1:A:806:ARG:HB3	2.03	0.57
1:A:443:ILE:HG22	1:A:592:MET:HG3	1.86	0.57
1:A:799:PRO:O	1:A:800:LYS:HB2	2.05	0.57
1:A:536:LYS:O	1:A:536:LYS:HD3	2.05	0.56
1:A:821:ALA:N	1:A:822:PRO:HD2	2.20	0.56
1:A:788:ILE:O	1:A:791:TYR:CD2	2.56	0.56
1:A:170:LEU:HB2	1:A:173:GLN:NE2	2.21	0.56
1:A:325:ILE:H	1:A:325:ILE:HD12	1.70	0.56
1:A:787:ASN:C	1:A:789:ALA:N	2.57	0.56
1:A:347:MET:HA	1:A:558:ASN:HD21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:LEU:HA	1:A:865:TRP:O	2.06	0.56
1:A:234:PHE:HB3	1:A:238:THR:HG21	1.87	0.56
1:A:713:TRP:CH2	1:A:723:PRO:HG3	2.40	0.56
1:A:147:TYR:HD1	1:A:147:TYR:N	2.04	0.55
1:A:410:PHE:CD1	1:A:410:PHE:N	2.74	0.55
1:A:663:ILE:HD13	1:A:683:MET:HE3	1.89	0.55
1:A:781:SER:O	1:A:831:TYR:O	2.24	0.55
1:A:818:ASN:O	1:A:822:PRO:HD3	2.06	0.55
1:A:818:ASN:HA	1:A:822:PRO:HG3	1.88	0.55
1:A:434:PHE:CZ	1:A:460:GLY:HA2	2.40	0.55
1:A:832:VAL:HG22	1:A:847:ALA:HB2	1.87	0.55
1:A:163:SER:OG	1:A:166:ILE:HG13	2.07	0.55
1:A:403:ARG:HG2	1:A:403:ARG:O	2.05	0.55
1:A:830:VAL:CG1	1:A:831:TYR:H	2.17	0.55
1:A:857:LEU:HD23	1:A:857:LEU:H	1.72	0.55
1:A:198:LEU:HD12	1:A:233:ILE:HD11	1.88	0.55
1:A:701:PHE:CE1	1:A:709:ALA:HB3	2.42	0.55
1:A:303:LEU:HD23	1:A:323:TYR:HB2	1.87	0.54
1:A:128:GLN:HG2	1:A:130:LYS:HG3	1.88	0.54
1:A:249:ARG:HD2	1:A:251:LYS:HE3	1.89	0.54
1:A:472:PRO:HA	1:A:475:ILE:HD12	1.90	0.54
1:A:593:ALA:HA	1:A:670:MET:HE3	1.88	0.54
1:A:459:ASN:HD22	1:A:459:ASN:N	2.02	0.54
1:A:195:LYS:O	1:A:199:MET:HB2	2.07	0.54
1:A:719:ARG:HG3	1:A:720:TYR:N	2.22	0.54
1:A:338:ARG:HG3	1:A:340:PHE:CE1	2.43	0.53
1:A:653:LYS:HD2	1:A:656:ARG:HH12	1.73	0.53
1:A:685:ARG:HG2	1:A:686:GLU:H	1.72	0.53
1:A:832:VAL:H	1:A:847:ALA:HA	1.73	0.53
1:A:524:ASP:HA	1:A:527:LYS:HB2	1.90	0.53
1:A:767:PHE:HA	1:A:770:GLU:HG2	1.90	0.53
1:A:193:ASN:ND2	1:A:195:LYS:HB2	2.22	0.53
1:A:810:THR:HG21	1:A:845:CYS:O	2.09	0.53
1:A:171:GLN:HG2	1:A:177:GLU:OE2	2.08	0.53
1:A:4:PHE:CE2	1:A:103:TYR:HA	2.44	0.53
1:A:790:LYS:O	1:A:792:ASP:N	2.42	0.53
1:A:594:LEU:O	1:A:597:ILE:HG22	2.09	0.53
1:A:164:ILE:HG13	3:A:963:HOH:O	2.07	0.52
1:A:897:LEU:HD12	1:A:897:LEU:H	1.73	0.52
1:A:647:TRP:C	1:A:647:TRP:CD1	2.82	0.52
1:A:312:LEU:HD12	1:A:320:TYR:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ARG:HH22	1:A:717:GLY:H	1.57	0.52
1:A:42:PRO:O	1:A:45:GLN:HG2	2.09	0.52
1:A:759:SER:O	1:A:762:GLU:HG2	2.09	0.52
1:A:836:ARG:HG3	1:A:867:ASP:HA	1.92	0.52
1:A:186:ILE:N	1:A:186:ILE:HD12	2.25	0.52
1:A:214:THR:HG21	1:A:273:TYR:CD2	2.37	0.52
1:A:263:ILE:N	1:A:263:ILE:HD12	2.25	0.52
1:A:416:TYR:O	1:A:420:ILE:HD12	2.10	0.52
1:A:772:ARG:HH11	1:A:772:ARG:HG3	1.74	0.52
1:A:834:PRO:CB	1:A:867:ASP:HB3	2.40	0.52
1:A:577:TYR:CD1	1:A:577:TYR:N	2.78	0.52
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.45	0.52
1:A:115:ILE:HD11	1:A:221:PHE:HE1	1.75	0.52
1:A:443:ILE:HD12	1:A:595:GLN:HB2	1.92	0.52
1:A:104:ASP:OD2	1:A:107:LYS:HG3	2.10	0.51
1:A:410:PHE:HB3	1:A:683:MET:HG2	1.91	0.51
1:A:82:ALA:HB3	3:A:935:HOH:O	2.08	0.51
1:A:64:ASN:O	1:A:67:ASP:HB2	2.10	0.51
1:A:178:VAL:O	1:A:183:ILE:HD11	2.11	0.51
1:A:218:VAL:O	1:A:223:ILE:HG13	2.09	0.51
1:A:303:LEU:HD23	1:A:323:TYR:CA	2.40	0.51
1:A:604:TYR:HD1	1:A:605:LEU:HD23	1.75	0.51
1:A:618:LEU:HB3	1:A:626:TYR:O	2.11	0.51
1:A:796:PHE:HB3	1:A:797:PRO:HD2	1.93	0.50
1:A:869:THR:O	1:A:873:GLU:HG3	2.10	0.50
1:A:169:LYS:HB2	1:A:175:GLY:HA3	1.92	0.50
1:A:6:LEU:HB2	1:A:18:ARG:O	2.11	0.50
1:A:309:ILE:HD13	1:A:309:ILE:O	2.11	0.50
1:A:604:TYR:CD1	1:A:605:LEU:HD23	2.46	0.50
1:A:173:GLN:H	1:A:173:GLN:HE21	1.60	0.50
1:A:273:TYR:OH	1:A:340:PHE:HB2	2.11	0.50
1:A:784:SER:HA	1:A:829:LYS:HA	1.94	0.50
1:A:193:ASN:OD1	1:A:196:GLU:HG3	2.12	0.50
1:A:402:ASN:HA	1:A:886:ALA:O	2.12	0.50
1:A:434:PHE:HE1	1:A:442:TYR:OH	1.94	0.50
1:A:461:MET:HE1	1:A:581:ARG:HD2	1.92	0.50
1:A:699:GLY:O	1:A:753:LEU:HD22	2.12	0.50
1:A:793:VAL:C	1:A:795:GLY:H	2.13	0.50
1:A:819:ILE:HG22	1:A:819:ILE:O	2.12	0.50
1:A:736:SER:HA	1:A:782:VAL:O	2.12	0.49
1:A:119:SER:O	1:A:310:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:GLU:HG3	1:A:687:ALA:H	1.78	0.49
1:A:368:ILE:HG22	1:A:369:ILE:N	2.27	0.49
1:A:112:ASN:HD22	1:A:113:PHE:N	2.10	0.49
1:A:353:ILE:HG13	1:A:354:GLN:O	2.13	0.49
1:A:411:ASP:O	1:A:683:MET:HA	2.12	0.49
1:A:464:TYR:H	1:A:464:TYR:HD1	1.60	0.49
1:A:5:TYR:HA	1:A:19:TYR:HB2	1.94	0.49
1:A:205:TRP:CZ3	1:A:242:LEU:O	2.63	0.49
1:A:459:ASN:H	1:A:459:ASN:ND2	2.10	0.49
1:A:606:ASN:HB2	1:A:611:THR:OG1	2.13	0.49
1:A:62:PHE:O	1:A:63:ALA:HB3	2.12	0.49
1:A:245:HIS:HE1	3:A:915:HOH:O	1.96	0.49
1:A:514:LEU:H	1:A:541:MET:CE	2.25	0.49
1:A:551:ALA:O	1:A:554:THR:HG22	2.13	0.49
1:A:820:ASP:C	1:A:822:PRO:HD2	2.33	0.48
1:A:85:MET:HG3	1:A:87:ASP:O	2.12	0.48
1:A:186:ILE:CD1	1:A:186:ILE:H	2.26	0.48
1:A:703:THR:HG22	1:A:707:ARG:HH11	1.79	0.48
1:A:819:ILE:O	1:A:820:ASP:HB2	2.12	0.48
1:A:186:ILE:H	1:A:186:ILE:HD12	1.77	0.48
1:A:771:PHE:HZ	1:A:871:LEU:HD13	1.77	0.48
1:A:402:ASN:OD1	1:A:888:LYS:HE2	2.14	0.48
1:A:533:LEU:HB3	1:A:538:LEU:HG	1.96	0.48
1:A:403:ARG:HH11	1:A:888:LYS:HB2	1.78	0.48
1:A:514:LEU:H	1:A:541:MET:HE1	1.79	0.48
1:A:354:GLN:HG3	3:A:936:HOH:O	2.13	0.48
1:A:300:VAL:HG23	1:A:301:GLY:H	1.78	0.47
1:A:504:HIS:C	1:A:506:PRO:HD3	2.34	0.47
1:A:689:ALA:HB1	1:A:711:ASN:O	2.14	0.47
1:A:116:GLU:HG3	1:A:324:ASN:ND2	2.20	0.47
1:A:329:TYR:O	1:A:332:LEU:HB2	2.14	0.47
1:A:553:MET:HG3	1:A:554:THR:N	2.29	0.47
1:A:595:GLN:HA	3:A:962:HOH:O	2.13	0.47
1:A:642:ARG:O	1:A:643:ASP:HB2	2.14	0.47
1:A:6:LEU:HD21	1:A:20:ILE:HG12	1.96	0.47
1:A:843:ASP:O	1:A:844:LYS:HG3	2.14	0.47
1:A:883:PHE:N	1:A:883:PHE:CD1	2.79	0.47
1:A:233:ILE:C	1:A:234:PHE:HD1	2.17	0.47
1:A:796:PHE:CB	1:A:797:PRO:HD2	2.44	0.47
1:A:296:PHE:C	1:A:296:PHE:HD1	2.18	0.47
1:A:71:TRP:O	1:A:74:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:HG23	1:A:354:GLN:HE21	1.80	0.47
1:A:489:MET:CG	1:A:553:MET:HB3	2.44	0.47
1:A:117:VAL:HG22	1:A:133:ILE:HA	1.96	0.47
1:A:181:GLU:OE1	1:A:181:GLU:N	2.48	0.47
1:A:20:ILE:CG2	1:A:24:GLY:HA2	2.44	0.47
1:A:24:GLY:HA3	1:A:107:LYS:HE3	1.97	0.47
1:A:597:ILE:CB	1:A:667:PHE:HE1	2.20	0.47
1:A:188:TYR:HE1	1:A:190:PRO:CG	2.18	0.46
1:A:536:LYS:C	1:A:536:LYS:HD3	2.35	0.46
1:A:214:THR:HG23	1:A:271:LEU:O	2.15	0.46
1:A:489:MET:HG3	1:A:553:MET:HB3	1.96	0.46
1:A:836:ARG:NH1	1:A:865:TRP:HA	2.30	0.46
1:A:597:ILE:HB	1:A:667:PHE:CE1	2.32	0.46
1:A:667:PHE:CD2	1:A:681:MET:CB	2.99	0.46
1:A:679:HIS:O	1:A:681:MET:N	2.47	0.46
1:A:876:PHE:O	1:A:880:LEU:HB2	2.14	0.46
1:A:791:TYR:OH	1:A:802:PRO:HD3	2.15	0.46
1:A:815:ILE:HA	1:A:815:ILE:HD12	1.72	0.46
1:A:836:ARG:HH11	1:A:865:TRP:HA	1.80	0.46
1:A:167:ALA:HA	1:A:176:ASP:HB2	1.97	0.46
1:A:643:ASP:O	1:A:646:HIS:HB3	2.16	0.46
1:A:321:ILE:O	1:A:325:ILE:HD12	2.15	0.45
1:A:464:TYR:N	1:A:464:TYR:CD1	2.85	0.45
1:A:763:TYR:CD1	1:A:763:TYR:C	2.89	0.45
1:A:249:ARG:CD	1:A:251:LYS:HE3	2.45	0.45
1:A:254:GLU:O	1:A:257:TYR:HD2	1.99	0.45
1:A:457:SER:HB3	1:A:459:ASN:ND2	2.31	0.45
1:A:821:ALA:N	1:A:822:PRO:CD	2.80	0.45
1:A:899:ASP:C	1:A:901:PHE:H	2.20	0.45
1:A:125:GLU:HB2	1:A:128:GLN:NE2	2.30	0.45
1:A:332:LEU:HA	1:A:332:LEU:HD13	1.67	0.45
1:A:747:GLU:HB3	1:A:763:TYR:CE2	2.51	0.45
1:A:291:ASP:HB2	1:A:292:TYR:H	1.49	0.45
1:A:405:LYS:O	1:A:690:GLY:HA2	2.16	0.45
1:A:751:ARG:NE	1:A:763:TYR:HD2	2.15	0.45
1:A:431:ALA:HB2	1:A:464:TYR:CD1	2.51	0.45
1:A:455:SER:O	1:A:462:MET:HA	2.15	0.45
1:A:402:ASN:ND2	1:A:403:ARG:H	2.14	0.45
1:A:597:ILE:HD12	1:A:600:LYS:HB2	1.99	0.45
1:A:253:ILE:O	1:A:254:GLU:HG3	2.16	0.45
1:A:415:LEU:O	1:A:416:TYR:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:LYS:O	1:A:845:CYS:HB3	2.16	0.45
1:A:163:SER:HB3	1:A:166:ILE:HD12	1.99	0.44
1:A:169:LYS:HB2	1:A:175:GLY:CA	2.48	0.44
1:A:763:TYR:HD1	1:A:763:TYR:C	2.21	0.44
1:A:143:ASP:O	1:A:144:ASP:HB3	2.17	0.44
1:A:533:LEU:HD12	1:A:537:SER:HB2	1.99	0.44
1:A:5:TYR:HA	1:A:19:TYR:CB	2.48	0.44
1:A:430:ILE:HG23	1:A:430:ILE:O	2.17	0.44
1:A:491:ALA:HA	1:A:494:ARG:HH21	1.82	0.44
1:A:686:GLU:O	1:A:715:MET:HA	2.17	0.44
1:A:771:PHE:O	1:A:774:LEU:HG	2.16	0.44
1:A:322:SER:O	1:A:326:ILE:HG12	2.17	0.44
1:A:578:TYR:CG	1:A:579:ASP:N	2.85	0.44
1:A:641:PHE:HA	1:A:646:HIS:CE1	2.52	0.44
1:A:644:THR:HG23	1:A:645:ASN:H	1.82	0.44
1:A:18:ARG:NH2	1:A:210:PRO:O	2.51	0.44
1:A:153:ASN:HB2	1:A:192:ASP:O	2.18	0.44
1:A:422:GLN:HB2	1:A:422:GLN:HE21	1.60	0.44
1:A:497:GLU:OE1	1:A:497:GLU:HA	2.18	0.44
1:A:692:PRO:O	1:A:693:LEU:CB	2.65	0.44
1:A:695:SER:HB2	1:A:754:GLN:O	2.18	0.44
1:A:158:ASN:N	1:A:158:ASN:HD22	2.15	0.44
1:A:165:GLU:H	1:A:165:GLU:CD	2.20	0.44
1:A:247:LYS:HB3	1:A:266:PHE:CD2	2.52	0.43
1:A:538:LEU:O	1:A:540:GLU:N	2.45	0.43
1:A:433:THR:CG2	1:A:434:PHE:N	2.80	0.43
1:A:686:GLU:HG3	1:A:687:ALA:N	2.33	0.43
1:A:247:LYS:O	1:A:266:PHE:HB2	2.19	0.43
1:A:137:THR:OG1	1:A:324:ASN:HB3	2.18	0.43
1:A:457:SER:HA	1:A:458:PRO:HD3	1.79	0.43
1:A:112:ASN:ND2	1:A:112:ASN:C	2.71	0.43
1:A:20:ILE:HG23	1:A:24:GLY:HA2	1.99	0.43
1:A:370:PHE:CD1	1:A:370:PHE:C	2.92	0.43
1:A:406:TYR:HB3	1:A:629:ALA:HB3	1.99	0.43
1:A:724:LYS:HB3	1:A:724:LYS:NZ	2.34	0.43
1:A:692:PRO:HG3	1:A:713:TRP:CZ2	2.54	0.43
1:A:636:VAL:HG12	1:A:636:VAL:O	2.17	0.43
1:A:647:TRP:O	1:A:650:PHE:N	2.52	0.43
1:A:741:VAL:HG13	1:A:876:PHE:HD1	1.83	0.43
1:A:303:LEU:HD21	1:A:319:ARG:HG3	2.01	0.43
1:A:254:GLU:HB3	1:A:255:ASN:H	1.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASP:CG	1:A:107:LYS:HG3	2.40	0.42
1:A:253:ILE:CG2	1:A:254:GLU:N	2.46	0.42
1:A:367:ALA:O	1:A:371:ASN:ND2	2.52	0.42
1:A:402:ASN:CG	1:A:403:ARG:H	2.22	0.42
1:A:457:SER:HB3	1:A:459:ASN:HD21	1.84	0.42
1:A:738:PRO:HG3	1:A:780:ALA:O	2.18	0.42
1:A:798:GLY:HA2	1:A:799:PRO:HD2	1.66	0.42
1:A:221:PHE:CD1	1:A:221:PHE:C	2.92	0.42
1:A:503:LEU:O	1:A:506:PRO:HG3	2.19	0.42
1:A:702:TRP:CD1	1:A:702:TRP:N	2.87	0.42
1:A:417:PRO:O	1:A:421:ARG:HG3	2.18	0.42
1:A:464:TYR:HD1	1:A:464:TYR:N	2.16	0.42
1:A:751:ARG:HE	1:A:763:TYR:HD2	1.68	0.42
1:A:776:TYR:CE1	1:A:777:ILE:HG13	2.54	0.42
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.87	0.42
1:A:240:LYS:NZ	1:A:248:THR:HG22	2.34	0.42
1:A:420:ILE:HD11	1:A:586:ILE:HD13	2.01	0.42
1:A:653:LYS:HD2	1:A:653:LYS:HA	1.87	0.42
1:A:731:GLU:HB3	1:A:734:LYS:HD2	2.01	0.42
1:A:74:ARG:HA	3:A:926:HOH:O	2.18	0.42
1:A:406:TYR:CB	1:A:629:ALA:HB3	2.49	0.42
1:A:818:ASN:CA	1:A:822:PRO:HG3	2.50	0.42
1:A:139:TYR:CE1	1:A:141:SER:HA	2.54	0.42
1:A:475:ILE:HG13	1:A:475:ILE:H	1.70	0.42
1:A:731:GLU:CB	1:A:734:LYS:HD2	2.50	0.42
1:A:145:ARG:HE	1:A:185:LYS:HD2	1.85	0.42
1:A:201:TYR:O	1:A:204:PHE:HB3	2.19	0.42
1:A:296:PHE:O	1:A:296:PHE:HD1	2.03	0.42
1:A:466:ASP:CG	1:A:467:ARG:H	2.23	0.42
1:A:846:ILE:CG2	1:A:847:ALA:N	2.80	0.42
1:A:514:LEU:HD12	1:A:514:LEU:N	2.35	0.42
1:A:486:LYS:HB2	1:A:556:GLN:HG3	2.02	0.42
1:A:774:LEU:HD23	1:A:774:LEU:N	2.35	0.42
1:A:818:ASN:O	1:A:819:ILE:HB	2.20	0.42
1:A:831:TYR:CD2	1:A:850:SER:HA	2.54	0.42
1:A:47:THR:HB	1:A:48:LYS:O	2.20	0.41
1:A:797:PRO:HB2	1:A:798:GLY:H	1.76	0.41
1:A:881:GLU:OE1	1:A:891:TYR:HE2	2.03	0.41
1:A:893:LYS:HG2	1:A:894:LYS:O	2.19	0.41
1:A:4:PHE:HA	1:A:97:TYR:CE2	2.54	0.41
1:A:218:VAL:CG1	1:A:219:GLU:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:VAL:HA	1:A:455:SER:OG	2.19	0.41
1:A:167:ALA:HA	1:A:176:ASP:OD2	2.20	0.41
1:A:182:ILE:O	1:A:185:LYS:HB2	2.20	0.41
1:A:198:LEU:O	1:A:199:MET:C	2.59	0.41
1:A:38:PHE:CE1	1:A:49:TYR:CD2	3.09	0.41
1:A:517:ASP:OD1	1:A:519:ARG:NE	2.53	0.41
1:A:460:GLY:O	1:A:461:MET:HE2	2.20	0.41
1:A:125:GLU:HB2	1:A:128:GLN:CD	2.40	0.41
1:A:420:ILE:HG21	1:A:475:ILE:HD11	2.02	0.41
1:A:528:GLU:C	1:A:530:ILE:N	2.71	0.41
1:A:765:LYS:O	1:A:768:GLU:HB3	2.20	0.41
1:A:224:PRO:HA	1:A:263:ILE:HD13	2.02	0.41
1:A:125:GLU:HA	1:A:126:PRO:HD3	1.94	0.41
1:A:461:MET:CE	1:A:581:ARG:HD2	2.51	0.41
1:A:221:PHE:CD1	1:A:222:ASP:N	2.89	0.41
1:A:647:TRP:CG	1:A:648:VAL:N	2.88	0.41
1:A:766:GLU:O	1:A:769:LYS:HB3	2.21	0.41
1:A:842:GLY:O	1:A:843:ASP:HB2	2.21	0.41
1:A:205:TRP:O	1:A:209:THR:N	2.54	0.41
1:A:788:ILE:HG22	1:A:791:TYR:CB	2.47	0.41
1:A:830:VAL:HG12	1:A:847:ALA:HB1	2.02	0.41
1:A:170:LEU:HD22	1:A:170:LEU:N	2.36	0.41
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.95	0.41
1:A:303:LEU:HD23	1:A:323:TYR:HA	2.02	0.41
1:A:52:ILE:HD12	1:A:381:PRO:HD3	2.03	0.40
1:A:538:LEU:HA	1:A:541:MET:HB3	2.02	0.40
1:A:559:ARG:HD3	1:A:559:ARG:HA	1.90	0.40
1:A:719:ARG:CG	1:A:720:TYR:N	2.84	0.40
1:A:730:LEU:HD23	1:A:730:LEU:HA	1.86	0.40
1:A:848:TRP:HB2	1:A:849:PRO:CD	2.51	0.40
1:A:250:VAL:O	1:A:251:LYS:HG3	2.21	0.40
1:A:297:GLU:OE1	1:A:338:ARG:NH1	2.54	0.40
1:A:422:GLN:NE2	1:A:679:HIS:O	2.54	0.40
1:A:534:SER:N	3:A:905:HOH:O	2.53	0.40
1:A:599:ARG:O	1:A:603:GLU:HB2	2.21	0.40
1:A:629:ALA:O	1:A:630:ASP:C	2.60	0.40
1:A:733:GLN:O	1:A:734:LYS:C	2.60	0.40
1:A:347:MET:CE	1:A:358:VAL:HG13	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	901/903 (100%)	732 (81%)	128 (14%)	41 (5%)	<b>3</b> <b>9</b>

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	255	ASN
1	A	259	SER
1	A	300	VAL
1	A	381	PRO
1	A	451	SER
1	A	507	ASN
1	A	680	LEU
1	A	768	GLU
1	A	791	TYR
1	A	793	VAL
1	A	799	PRO
1	A	819	ILE
1	A	829	LYS
1	A	98	ASN
1	A	312	LEU
1	A	390	PRO
1	A	509	SER
1	A	622	THR
1	A	637	GLY
1	A	692	PRO
1	A	797	PRO
1	A	818	ASN
1	A	827	GLY
1	A	44	SER
1	A	291	ASP
1	A	832	VAL
1	A	102	LYS

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Mol	Chain	Res	Type
1	A	161	GLU
1	A	316	ASN
1	A	462	MET
1	A	804	HIS
1	A	834	PRO
1	A	845	CYS
1	A	24	GLY
1	A	523	SER
1	A	659	MET
1	A	735	SER
1	A	766	GLU
1	A	401	PRO
1	A	506	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	802/802 (100%)	675 (84%)	127 (16%)	<b>3</b> <b>9</b>

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	PHE
1	A	6	LEU
1	A	21	ASP
1	A	22	SER
1	A	23	ASN
1	A	44	SER
1	A	52	ILE
1	A	55	LYS
1	A	58	THR
1	A	61	LEU
1	A	70	GLN
1	A	86	ASP

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Mol	Chain	Res	Type
1	A	101	ILE
1	A	105	HIS
1	A	112	ASN
1	A	127	SER
1	A	147	TYR
1	A	158	ASN
1	A	164	ILE
1	A	173	GLN
1	A	184	ASP
1	A	195	LYS
1	A	197	LEU
1	A	199	MET
1	A	205	TRP
1	A	209	THR
1	A	214	THR
1	A	218	VAL
1	A	225	TYR
1	A	232	ASN
1	A	237	SER
1	A	238	THR
1	A	255	ASN
1	A	273	TYR
1	A	280	PHE
1	A	291	ASP
1	A	296	PHE
1	A	299	ASN
1	A	300	VAL
1	A	309	ILE
1	A	312	LEU
1	A	316	ASN
1	A	324	ASN
1	A	337	LYS
1	A	338	ARG
1	A	342	ASN
1	A	356	GLN
1	A	370	PHE
1	A	373	LEU
1	A	382	GLN
1	A	384	ARG
1	A	403	ARG
1	A	410	PHE
1	A	411	ASP

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Mol	Chain	Res	Type
1	A	412	LEU
1	A	418	SER
1	A	426	SER
1	A	428	GLU
1	A	430	ILE
1	A	433	THR
1	A	436	VAL
1	A	452	ASP
1	A	456	CYS
1	A	459	ASN
1	A	464	TYR
1	A	468	ASP
1	A	473	THR
1	A	501	GLU
1	A	505	ASN
1	A	507	ASN
1	A	514	LEU
1	A	519	ARG
1	A	520	PHE
1	A	524	ASP
1	A	528	GLU
1	A	541	MET
1	A	542	LEU
1	A	553	MET
1	A	556	GLN
1	A	559	ARG
1	A	562	LEU
1	A	575	PHE
1	A	589	PHE
1	A	594	LEU
1	A	595	GLN
1	A	618	LEU
1	A	631	LYS
1	A	639	SER
1	A	640	LYS
1	A	644	THR
1	A	646	HIS
1	A	647	TRP
1	A	658	ARG
1	A	665	ARG
1	A	667	PHE
1	A	684	ASP

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Mol	Chain	Res	Type
1	A	692	PRO
1	A	693	LEU
1	A	698	ILE
1	A	716	GLU
1	A	728	MET
1	A	731	GLU
1	A	763	TYR
1	A	767	PHE
1	A	768	GLU
1	A	769	LYS
1	A	773	GLN
1	A	791	TYR
1	A	793	VAL
1	A	796	PHE
1	A	804	HIS
1	A	809	LEU
1	A	815	ILE
1	A	823	GLN
1	A	824	VAL
1	A	834	PRO
1	A	845	CYS
1	A	855	THR
1	A	857	LEU
1	A	869	THR
1	A	871	LEU
1	A	872	LEU
1	A	880	LEU
1	A	884	THR
1	A	890	ASP
1	A	900	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	128	GLN
1	A	131	HIS
1	A	158	ASN
1	A	173	GLN
1	A	232	ASN
1	A	316	ASN
1	A	324	ASN

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Mol	Chain	Res	Type
1	A	333	GLN
1	A	354	GLN
1	A	356	GLN
1	A	422	GLN
1	A	459	ASN
1	A	481	GLN
1	A	676	ASN
1	A	773	GLN
1	A	787	ASN
1	A	812	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	5GP	A	904	-	22,26,26	2.64	9 (40%)	26,40,40	3.20	7 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5GP	A	904	-	-	0/6/26/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	904	5GP	O4'-C4'	2.61	1.50	1.45
2	A	904	5GP	C2'-C3'	2.95	1.61	1.53
2	A	904	5GP	O3'-C3'	3.06	1.50	1.43
2	A	904	5GP	C3'-C4'	3.20	1.61	1.53
2	A	904	5GP	C2-N1	3.33	1.41	1.35
2	A	904	5GP	C5'-C4'	3.72	1.63	1.51
2	A	904	5GP	C6-N1	4.34	1.40	1.33
2	A	904	5GP	O4'-C1'	5.46	1.48	1.41
2	A	904	5GP	C6-C5	5.56	1.51	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	904	5GP	C5-C6-N1	-11.84	106.62	123.48
2	A	904	5GP	C2-N3-C4	-3.80	110.72	115.16
2	A	904	5GP	C5'-C4'-C3'	-3.11	103.42	115.29
2	A	904	5GP	C4-C5-N7	-2.20	107.29	109.41
2	A	904	5GP	O4'-C4'-C5'	2.83	118.94	109.40
2	A	904	5GP	O5'-C5'-C4'	4.80	126.03	109.00
2	A	904	5GP	C6-N1-C2	7.05	126.20	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	903/903 (100%)	-0.33	9 (0%) 82 77	45, 73, 100, 100	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	MET	3.1
1	A	257	TYR	2.6
1	A	259	SER	2.6
1	A	507	ASN	2.5
1	A	826	GLU	2.4
1	A	114	ASP	2.1
1	A	323	TYR	2.1
1	A	301	GLY	2.0
1	A	324	ASN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	5GP	A	904	24/24	0.94	0.15	-0.54	70,72,74,74	4

## 6.5 Other polymers [i](#)

There are no such residues in this entry.